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L1      STRUCTURE UPLOADED

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L1                STR
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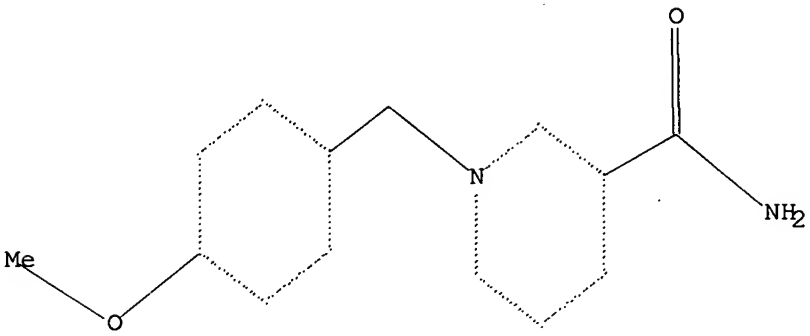


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Structure attributes must be viewed using STN Express query preparation.


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SAMPLE SEARCH INITIATED 12:08:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     957 TO ITERATE

100.0% PROCESSED     957 ITERATIONS                                  3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         17285 TO    20995
PROJECTED ANSWERS:                3 TO      163

L2             3 SEA SSS SAM L1

=> d scan l2
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=> d his

     (FILE 'HOME' ENTERED AT 12:07:23 ON 31 MAY 2005)

     FILE 'REGISTRY' ENTERED AT 12:07:32 ON 31 MAY 2005
L1             STRUCTURE UPLOADED
L2           3 S L1 SSS SAM
L3          32 S L1 SSS FULL

     FILE 'HCAPLUS' ENTERED AT 12:09:40 ON 31 MAY 2005

=> s l3
L4          22 L3

=> d l4 abs cbib hitstr 1-22

L4   ANSWER 1 OF 22  HCAPLUS  COPYRIGHT 2005 ACS on STN
AB   Structure-activity relationships for a recently discovered novel ribosome
     inhibitor (NRI) class of antibacterials were investigated.  Preliminary
     efforts to optimize protein synthesis inhibitory activity of the series
     through modification of positions 3 and 4 of the naphthyridine lead
     template resulted in the identification of several biochem. potent
     analogs.  A lack of corresponding whole cell antibacterial activity is
     thought to be a consequence of poor cellular penetration as evidenced by
     the enhancement of activity observed for a lead analog tested in the presence
     of a cell permeabilizing agent.
2004:403900  Document Number 141:99019  Novel inhibitors of bacterial protein
     synthesis: structure-activity relationships for 1,8-naphthyridine
     derivatives incorporating position 3 and 4 variants.  Clark, Richard F.;
     Wang, Sanyi; Ma, Zhenkun; Weitzberg, Moshe; Motter, Christopher; Tufano,
     Michael; Wagner, Rolf; Gu, Yu-Gui; Dandliker, Peter J.; Lerner, Claude G.;
     Chovan, Linda E.; Cai, Yingna; Black-Schaefer, Candace L.; Lynch, Linda;
     Kalvin, Douglas; Nilius, Angela M.; Pratt, Steve D.; Soni, Niru; Zhang,
     Tianyuan; Zhang, Xiaolin; Beutel, Bruce A. (Global Pharmaceutical Research
     and Development, Abbott Laboratories, Abbott Park, IL, 60064, USA).
     Bioorganic & Medicinal Chemistry Letters, 14(12), 3299-3302 (English)
     2004.  CODEN: BMCLE8.  ISSN: 0960-894X.  OTHER SOURCES: CASREACT
     141:99019.  Publisher: Elsevier Science B.V..
IT   779339-36-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and structure-activity relationships studies of
        1,8-naphthyridine derivs. as novel inhibitors of bacterial protein
        synthesis)
RN   779339-36-5  HCAPLUS
CN   1,8-Naphthyridine-3-carboxamide, 7-(3-amino-1-pyrrolidinyl)-1-[(2,4-
     dimethoxyphenyl)methyl]-6-fluoro-1,4-dihydro-4-oxo- (9CI)  (CA INDEX NAME)
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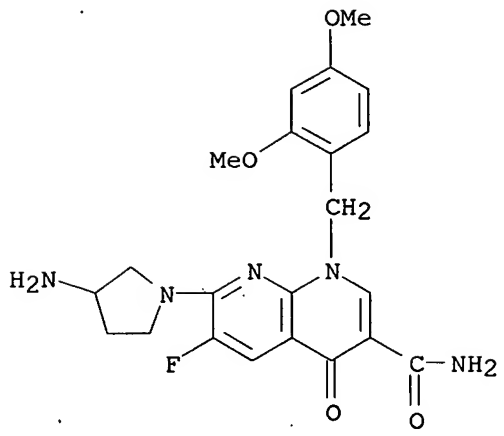
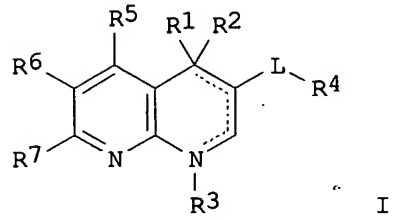


L4 ANSWER 2 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN
GI



I

AB The title compds. [I; one of R1 and R2 is absent or H, and the other = H, OH, NMe2, (un)substituted NH2; or R1 and R2 together = O; R3 = absent, alkyl, CH2CF3, OCH2CH:CH2, etc.; L = a bond, CO, (CH2)m (wherein m = 1-5); R4 = H, aryl, NH2, OH, etc.; R5 = H, alkyl, aryl, halo, etc.; R6 = H, halo, alkyl, CN, etc,; or R5 and R6 taken together = (un)substituted alkylene, heteroalkylene; R7 = halo, aryl, heteroaryl, etc.], useful for prophylaxis and treatment of bacterial infections, were prepared E.g., a multi-step synthesis of 7-[(3R)-3-aminopyrrolidin-1-yl]-6-fluoro-5-methyl-4-oxo-1,4-dihydro-1,8-naphthyridine-3-carboxylic acid, starting from 2,6-dichloro-5-fluoronicotinic acid (no data for intermediates), was given. The compds. I showed IC50 values in the range 0.01-40 μM against bacterial protein synthesis in S30 Streptococcus pneumoniae assay. The compns. comprising the compound I were claimed.

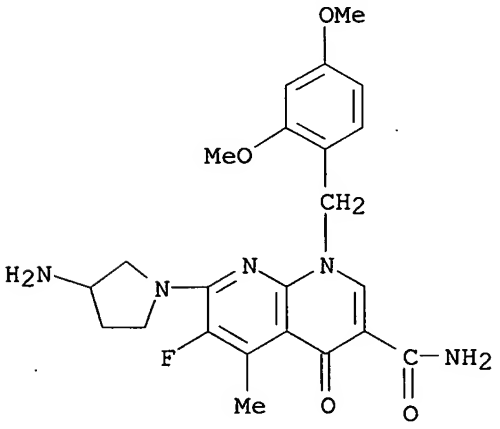
2003:991172 Document Number 140:42160 Preparation of naphthyridines as antibacterial compounds. Anderson, David; Beutel, Bruce; Bosse, Todd D.; Clark, Richard; Cooper, Curt; Dandliker, Peter; David, Caroline; Gu, Yu-Gui; Hansen, Todd Matthew; Hinman, Mira; Kalvin, Douglas; Larson, Daniel P.; Lynch, Linda; Ma, Zhenkun; Motter, Christopher; Palazzo, Fabio; Rosenberg, Teresa; Rehm, Tamara; Sanders, William; Tufano, Michael; Wagner, Rolf; Weitzberg, Moshe; Yong, Hong; Zhang, Tianyuan (USA). U.S. Pat. Appl. Publ. US 2003232818 A1 20031218, 118 pp. (English). CODEN: USXXCO. APPLICATION: US 2003-387318 20030312. PRIORITY: US 2002-PV363594

20020312.

IT **635306-36-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of naphthyridines as antibacterial compds.)

RN 635306-36-4 HCAPLUS

CN 1,8-Naphthyridine-3-carboxamide, 7-(3-amino-1-pyrrolidinyl)-1-[(2,4-dimethoxyphenyl)methyl]-6-fluoro-1,4-dihydro-5-methyl-4-oxo- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN

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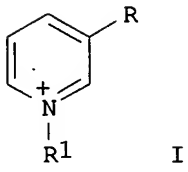

I

AB Novel agents acting as co-factors for replacement of NAD(P)+/NAD(P)H co-enzyme systems in enzymic redox reactions are disclosed. A composition for replacement or regeneration of an NAD(P)+/NAD(P)H system in redox processes comprising (a) a polymer matrix, (b) a catalyst precursor, (3) a cofactor, and (d) an enzyme is further disclosed. The NAD(P) mimics are I [R = CN, CONH2, CONHMe, CSNH2, COCH3, COOMe; R1 = CH2(CH2O)nYR2, ribose-YR2, or (X substituted)benzyl; Y = OP(:O)O, OBO2, OSO2, NHMe, (CH2)nNH, adenine, imidazole; R2 = H, Me, (OCH2CH2)n, (NCH2CH2)n, [N:P(OMe)2]n; X = OMe, CF3, (OCH2CH2)n, OP(:O)OR3; R3 = H, Me, (OCH2CH2)n, (NCH2CH2)n, [N:P(OMe)2]n; n = 1-2000] and salts thereof. Thus, I with R1 = benzyl and R = various substituents such as CONH2 as well as I with R1 = ribose 5'-methylphosphate and R = CONH2 were synthesized and studied.

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Both of these coAlc. dehydrogenase enzyme mimics were used by horse liver alc. dehydrogenase to reduce phenethylmethylketone to the corresponding alc. with >93% ee (S-enantiomer). The reduced mimics were produced in this reaction using [Cp*Rh(bpy)(H2O)](OTf)2 as a catalyst precursor and sodium formate as hydride source.

2002:716518 Document Number 137:228603 NAD(P) mimic for use in enzymic redox reactions. Fish, Richard H.; Kerr, John B.; Lo, Christine H. (The Regents of the University of California, USA). PCT Int. Appl. WO 2002072869 A2 20020919, 63 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2002-US7444 20020311. PRIORITY: US 2001-805726 20010312.

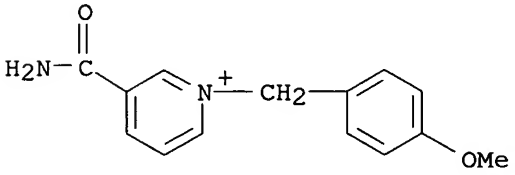
IT **459165-10-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(NAD(P) mimic for use in enzymic redox reactions)

RN 459165-10-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

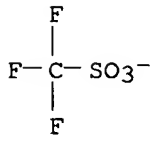
CM 1

CRN 175979-55-2
CMF C14 H15 N2 O2



CM 2

CRN 37181-39-8
CMF C F3 O3 S



L4 ANSWER 4 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN

AB The title compds. YAr+X- [I; Ar = 5-6 membered heteroaryl ring having a first ring N atom and optionally second or third ring N atoms, with the

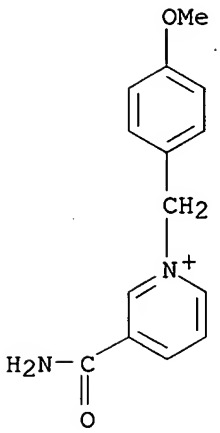
remaining ring atoms being C, O, or S, (provided the first N atom of Ar is a quaternary N and Ar is not thiazolium, oxazolium or imidazolium); Y is substituted on the first ring N atom (with the proviso that if Ar is pyrazole, indazole, triazole, benzotriazole, the second ring N atom is substituted with alkyl, alkoxycarbonylalkylene, aryl, etc.); Ar can be substituted on ring C atoms with aryl, carbamoyl, aralkyl, etc.; Y = CHR5R6 (R5 = H, alkyl, cycloalkyl, etc.; R6 = H, alkyl, alkenyl, etc.); X = a pharmaceutically acceptable anion, which may be absent if the compound provides a neutralizing salt], useful in treating or ameliorating certain fibrotic diseases or other indications linked to or associated with the formation of excess collagen, in an animal, including a human, were prepared Thus, refluxing 2-aminothiadiazole with 2-bromoacetamide in MeCN for 5 h afforded 5-amino-3-carbamoylmethyl-[1,3,4]thiadiazolium bromide. Assays to determine the activity of compds. I in breaking, reversing or inhibiting the formation of advanced glycosylation end products (AGEs) or AGE-mediated cross-links was presented (no data).

2002:675770 Document Number 137:216955 Method for treating fibrotic diseases or other indications using thiadiazolium, pyridinium and pyrimidinium salts. Wagle, Dilip; Gall, Martin; Bell, Stanley C.; Lavoie, Edmond J. (Alteon, Inc., USA). PCT Int. Appl. WO 2002067851 A2 20020906, 104 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-US49833 20011228. PRIORITY: US 2000-PV259294 20001229; US 2001-PV259238 20010102; US 2001-PV296246 20010606.

IT **63828-55-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

RN 63828-55-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L4 ANSWER 5 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

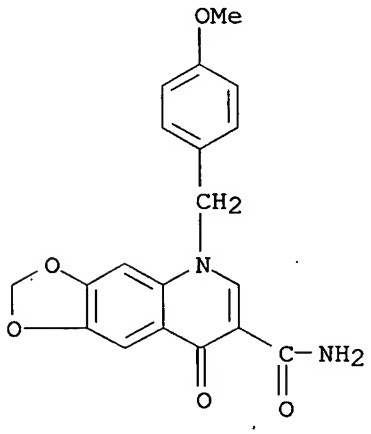
AB Title compds. I [n = 0 or 1; Y = NH, O, S, or alkylamine; R5 = CN, F, Cl, or Br; R6 = (un)substituted -cycloalkyl, -pyridinyl, -pyrimidinyl, -Ph, etc.; R1, R2 and R4 independently = H, OH, halo, CN, NO2, F3C, alkyl, amine, alkylamine, dialkylamine, R7X1(CH2)x- wherein x = 0-3, R7 = H, (un)substituted hydrocarbyl or heterocyclyl and X1 = O, CH2, OCO, CO, S, SO, SO2, NR8CO, NR8CO2, CONR9, CO2NR9, SO2NR10, NR11 or NR11NR11 wherein R8, R9, R10 and R11 independently = H, alkyl or alkoxyalkyl; R3 = group of formula X1R12(OH)p where p = 1-2 and R12 = alkylene, alkenylene or alkynylene chain, optionally interposed with a heteroatom or heterocyclic ring with the provision that when R12 = alkylene, R12 must be interposed with a heteroatom or heterocyclic ring and at least one (OH)p is on the alkylene chain between X1 and the interposed heteroatom or heterocyclic ring; group of formula R7(CH2)yX1(CH2)x where y = 0-5 and (CH2)y is optionally interposed by an X1 group; group of formula X1alkyl where alkyl is substituted by one or more Cl and/or CN; heterocyclic ring, etc.], or a pharmaceutically acceptable salt, pro-drug or solvate thereof are prepared and disclosed as antiproliferative agents. Thus, II was prepared in eight steps from benzylchloroformate and 2-methoxy-5-nitroaniline. I were evaluated as inhibitors of MAPK pathway and exhibited IC50 values typically lest than 0.5 μM, e.g., II possessed an IC50 = 0.0013μM. In cell proliferation assays, I had IC50 results typically less than 30μM with II giving an IC50 of 1.3 μM in HT29 human colon tumor cells. Methods for prevention of cancer comprising administering an effective amount of compound I are further claimed.

2002:428894 Document Number 137:20303 Preparation of substituted quinolines as antitumor agents. Boyle, Francis Thomas; Gibson, Keith Hopkinson; Foote, Kevin Michael (Astrazeneca AB, Swed.; Astrazeneca UK Limited). PCT Int.

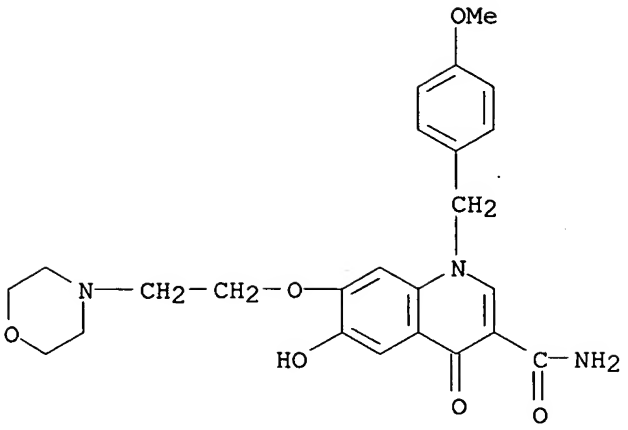
Appl. WO 2002044166 A1 20020606, 118 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-GB4737 20011026. PRIORITY: GB 2000-26744 20001102; GB 2000-26746 20001102; GB 2000-26747 20001102.

IT **423180-25-0P 433980-48-4P 433980-49-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation, inhibition of MAP kinase, and cellular antiproliferation activity of substituted quinolines as antitumor agents)

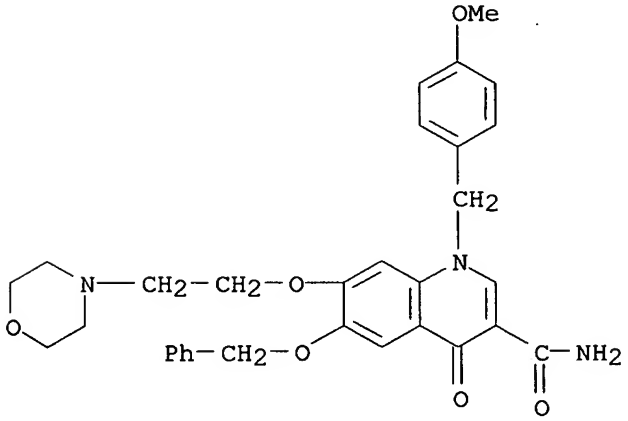
RN 423180-25-0 HCAPLUS
CN 1,3-Dioxolo[4,5-g]quinoline-7-carboxamide, 5,8-dihydro-5-[(4-methoxyphenyl)methyl]-8-oxo- (9CI) (CA INDEX NAME)



RN 433980-48-4 HCAPLUS
CN 3-Quinolinecarboxamide, 1,4-dihydro-6-hydroxy-1-[(4-methoxyphenyl)methyl]-7-[2-(4-morpholinyl)ethoxy]-4-oxo- (9CI) (CA INDEX NAME)



RN 433980-49-5 HCAPLUS
CN 3-Quinolinecarboxamide, 1,4-dihydro-1-[(4-methoxyphenyl)methyl]-7-[2-(4-morpholinyl)ethoxy]-4-oxo-6-(phenylmethoxy)- (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. I [R1, R2, R3, R4 independently H, HO, halogen, NC, O2N, F3C, (un)substituted C1-C3 alkyl, (un)substituted amino, saturated heterocyclyl containing two heteroatoms; R5 = NC, F, Cl, Br; R6 = divalent C1-C5 alkenyl, C3-C7 cycloalkyl, or heteroaryl moiety; R7 = AR8; A = bond, O, CO, S, SO, SO2, (un)substituted aminocarbonyl, (un)substituted carbonylamino, (un)substituted sulfonylamino, (un)substituted aminosulfonyl, (un)substituted amino; R8 = C1-C6 alkyl, C2-C6 alkenyl, C2-C6 alkynyl; R9 = (un)substituted C3-C7 divalent cycloalkyl; R10 = (un)substituted arylene, heteroarylene, heteroarylene N-oxide, C3-C10 cycloalkylene; X =

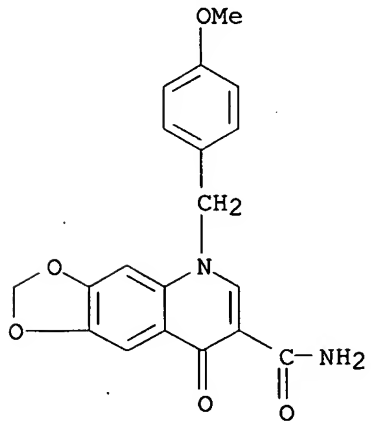
amino, (C1-C6)alkylamino, O, S, CH2; Y = amino, (C1-C6)alkylamino, O, S; Z = (un)substituted alkyl, alkylene, alkynylene, O, CO, COO, S, SO, SO2, (un)substituted aminocarbonyl, carbonylamino, sulfonylamino, aminosulfonyl, amino; n = 0,1; m and p independently 0-3; alternatively, R10Z(CH2)pR6R7 can be replaced with a heteroaryl or heterocyclyl-2,3-fused Ph ring] were prepared as inhibitors of MAP kinase for use as antitumor agents. E.g., 1-fluoro-4-nitrobenzene undergoes nucleophilic substitution with (2-hydroxyphenoxy)acetic acid followed by coupling of the acid with Me glycinate, reduction of the nitro group with Pd/C, and reaction of the ester with N-methylpiperazine to give the aminophenoxymethylcarbonylaminoa cetyl piperazine II. E.g., coupling of II with 4-chloro-6,7-dimethoxy-3-quinolinenitrile gave the example compound III. Biol. data was obtained for selected compds. Selected compds. inhibited MAP kinase with IC50 < 0.5 μM; for example, III gave an IC50 of 3.8 nM. In addition, selected compds. inhibited the proliferation of human colon cancer cells with IC50 < 30 μM; for example, III gave an IC50 of 1 μM.

2002:353433 Document Number 136:369616 Preparation of 3-cyano-4-arylaminoquinolines as inhibitors of MAP kinase for use as antitumor agents. Boyle, Francis Thomas; Gibson, Keith Hopkinson (Astrazeneca AB, Swed.; Astrazeneca UK Limited). PCT Int. Appl. WO 2002036570 A1 20020510, 149 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-GB4733 20011025. PRIORITY: GB 2000-26745 20001102; GB 2000-26747 20001102.

IT **423180-25-0P 423180-26-1P 423180-27-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediates; preparation of 4-arylamino-3-cyanoquinolines as inhibitors of MAP kinase for potential use as antitumor agents)

RN 423180-25-0 HCAPLUS

CN 1,3-Dioxolo[4,5-g]quinoline-7-carboxamide, 5,8-dihydro-5-[(4-methoxyphenyl)methyl]-8-oxo- (9CI) (CA INDEX NAME)



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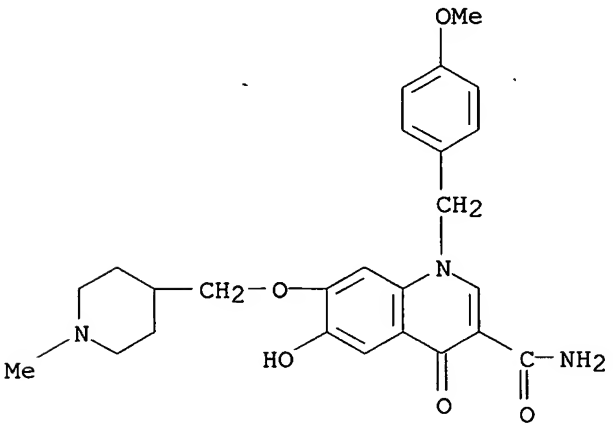
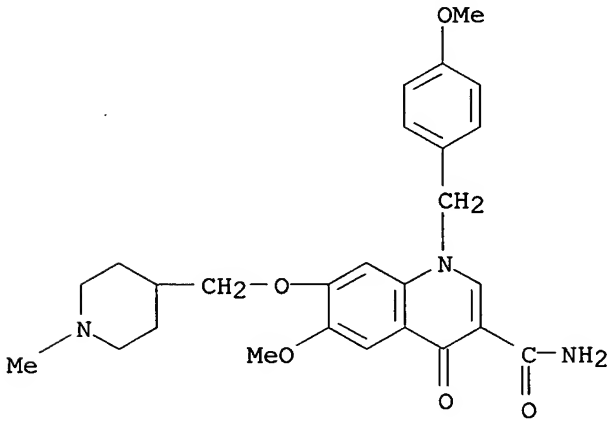
RN 423180-26-1 HCAPLUS
CN 3-Quinolinecarboxamide, 1,4-dihydro-6-hydroxy-1-[(4-methoxyphenyl)methyl]-7-[(1-methyl-4-piperidinyl)methoxy]-4-oxo- (9CI) (CA INDEX NAME)



RN 423180-27-2 HCAPLUS
CN 3-Quinolinecarboxamide, 1,4-dihydro-6-methoxy-1-[(4-methoxyphenyl)methyl]-7-[(1-methyl-4-piperidinyl)methoxy]-4-oxo- (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN
AB Second-order rate consts. and activation values were measured for the reactions with NaN3 of a series of 4-Y-substituted (Y = MeO, Me, H, Cl, and NO2) benzyl 3'-Z-substituted (Z = CN, CONH2, H, F, Ac) pyridinium chlorides in deuterium oxide. 3'-Cyanopyridine substrates reacted much faster than nicotinamide and pyridine substrates; in the pyridine series the 4-Me, 4-H, and 4-Cl benzyl analogs did not react for up to 6 mo at 96° in 1.7 M NaN3. The 3'-cyanopyridine substrates do not exhibit borderline kinetic behavior, but the nicotinamide substrates do. The Hammett plot is flat for the NaN3 reaction of 3'-cyanopyridine substrates and increasingly V-shaped for the nicotinamide and pyridine substrates. The values of βLG (four-point plot) for the NaN3 reaction of the

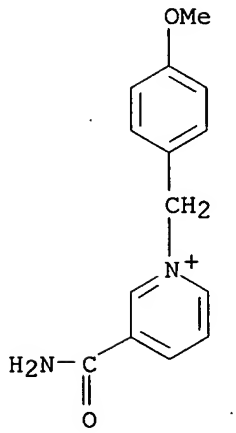
4-MeO benzyl substrates is -1.45, which is usually interpreted as being a very "late" activated complex. Two-point Bronsted "plots" for the other benzyl derivs. and for two N-methylpyridinium ions give values of βLG in the same range. The second-order rate constant and activation values for N-methyl-3'-cyanopyridinium iodide are within the same range as those for the benzyl substrates. For the hydrolysis reaction, the Hammett plot is linear for 3'-cyanopyridine substrates (ρ+ = -1.24) and flat for the nicotinamide substrates. The extent of hydrolysis of 0.005-0.05 M solns. of the 3'-cyanopyridinie substrates depended on the initial concentration of substrate, and hydrolysis was slowed significantly or stopped completely in the presence of exogenous 3-cyanopyridine. These results show that an equilibrium is established among the products for the 4-MeO, 4-Me, 4-H, and 4-Cl substrates; the 4-NO2 substrate reacted too slowly to discern any difference. Data for the extent of hydrolysis were fitted by an equation derived assuming the equilibrium Despite this limitation on a classic test of mechanism, the rates and ρ values are consistent with direct displacement by solvent and not with a unimol. process. These results, which are rationalized in terms of the Pross-Shaik model, suggest that there are no ion-dipole complex intermediates in the benzyl series and show that borderline kinetic behavior is a function of leaving group ability and is not necessarily related to a change in mechanism. A computational approach was used to evaluate anomalous βLG values for the hydrolysis and nucleophilic substitution reactions of the methylpyridinium ion substrates. It was found that neither the Nu-substrate bond lengths nor the difference in charge matched the βLG values. The value of ΔΔS.thermod. of -15 gibbs/mol between (4-methoxybenzyl)-3'-cyanopyridinium chloride and the corresponding dimethylsulfonium chloride in the NaN3 reaction, which is the result of the solvation of the pyridine at the transition state and the lack of solvation of SMe2, is used to argue that the source of NAD+ glycohydrolase "catalysis" of NAD+ bond cleavage is the result of desolvation of the leaving group upon binding.

1996:619241 Document Number 125:300276 Reactions of Charged Substrates. 5. The Solvolysis and Sodium Azide Substitution Reactions of Benzylpyridinium Ions in Deuterium Oxide. Buckley, Neil; Oppenheimer, Norman J. (Department of Pharmaceutical Chemistry, University of California, San Francisco, CA, 94143-0446, USA). Journal of Organic Chemistry, 61(21), 7360-7372 (English) 1996. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

IT **63828-55-7**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

RN 63828-55-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl^-

L4 ANSWER 8 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN

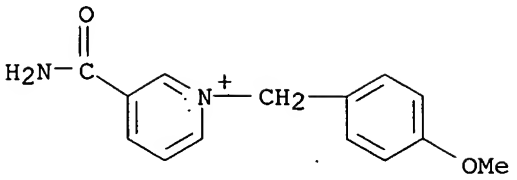
AB The relative rates for the gas-phase dissociation RX+ → R+ + X° of five (4-Y-substituted benzyl)dimethysulfoniums (Y = MeO, Me, H, Cl, and NO2) and 24 (4-Y-substituted benzyl)-3'-Z-pyridiniums (complete series for Z = CN, Cl, CONH2, and H, and 4-methoxy- and 4-nitrobenzyls for Z = F and CH3CO) were measured using liquid secondary ion mass spectrometry. The Hammett plot (vs δΔG0 or σ+) is linear for the sulfoniums, but plots for the four pyridinium series have a drastic break between the 4-Cl and 4-NO2 substrates. Broensted-like plots for the pyridiniums show a strong leaving group effect only for 4-nitrobenzyls. An anal. of these linear free energy relations with supporting evidence from semiempirical computations suggests that collisionally activated pyridinium substrates dissociate through two pathways, direct dissociation and an ion-neutral complex intermediate. Comparison of these results with results for the solution reactions of some of these compds. shows that the mechanism is different in the gas and solution phases. Sufficient exptl. data are not available to assign a mechanism for dissociation to the sulfonium series, but computational results show characteristics of a direct dissociative mechanism.

1996:191937 Document Number 124:316412 Reactions of Charged Substrates. 4. The Gas-Phase Dissociation of (4-Substituted benzyl)dimethylsulfoniums and -pyridiniums. Buckley, Neil; Maltby, David; Burlingame, Alma L.; Oppenheimer, Norman J. (School of Pharmacy, University of California, San Francisco, CA, 94143-0446, USA). Journal of Organic Chemistry, 61(8), 2753-62 (English) 1996. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

IT **175979-55-2**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

RN 175979-55-2 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 9 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN

AB Various NADH model compds., 1-(R-benzyl)-1,4-dihydronicotinamide (R-BNAH: R = 4-MeO, 4-Me, H, 4-Cl2, 2,4-Cl2) and 10-methyl-9,10-dihydroacridine (AcrH2), form complexes with metalloporphyrins (FeTPPClO4, FeTPPCl, MnTPPClO4, and ZnTPP; TPP: tetraphenylporphyrin) in CH2Cl2 or CHCl3. For the BNAH-ZnTPP system, the stoichiometry of the complex formation is 1:1 with the formation constant K = 50 dm3 mol-1 in CH2Cl2 at 298 K. In the BNAH-MTPPClO4 system (M = Fe and Mn), both 1:1 and 2:1 complexes are formed depending on the ratio of BNAH to MTPPClO4. The formation constant becomes larger as the donor ability of NADH model compds. increases. Both the five-coordinate FeTPP(BNAH)+ and six-coordinate FeTPP(BNAH)2+ complexes are high-spin (S = 5/2) species. The complex formation of the reduced metalloporphyrin (FeTPP and MnTPP) with BNAH was also investigated by the technique of cyclic voltammetry, which revealed that the reduced iron porphyrin FeTPP also forms a bis-coordination complex with BNAH, but the MnTPP forms only a mono-ligand adduct with BNAH. NADH model compds. act as two-electron donors in electron-transfer reactions with FeTPPClO4 in the presence of O in MeCN, when the overall rates are determined by the rates of electron transfer from R-BNAH to FeTPP+ together with the competition between the back electron transfer from FeTPP to R-BNAH+• and the deprotonation of BNAH+•.

1990:423470 Document Number 113:23470 Complex formation between NADH model compounds and metalloporphyrins. Fukuzumi, Shunichi; Kondo, Yuji; Mochizuki, Seiji; Tanaka, Toshio (Faculty English, Osaka University, Suita, 565, Japan). Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (11), 1753-61 (English) 1989. CODEN: JCPKBH. ISSN: 0300-9580.

IT **127747-91-5**
RL: PRP (Properties)
(formation constant of)

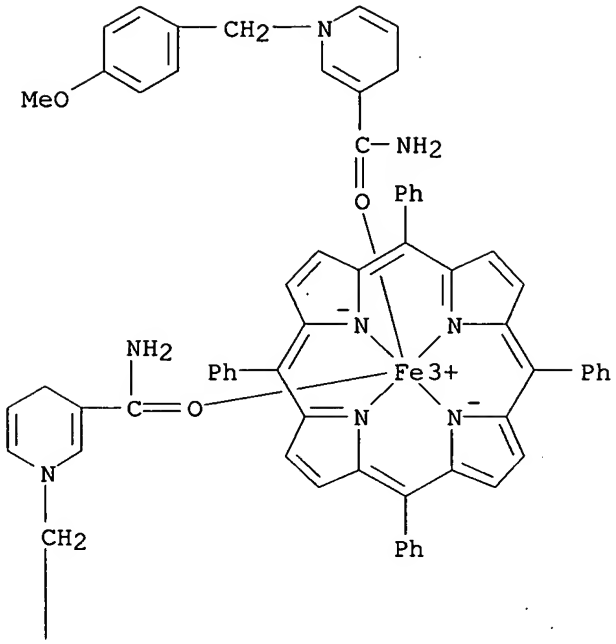
RN 127747-91-5 HCAPLUS

CN Iron(1+), bis[1,4-dihydro-1-[(4-methoxyphenyl)methyl]-3-pyridinecarboxamide-O3][5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (OC-6-12)-, perchlorate (9CI) (CA INDEX NAME)

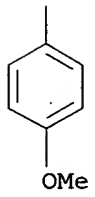
CM 1

CRN 127747-90-4
CMF C72 H60 Fe N8 O4
CCI CCS

PAGE 1-A

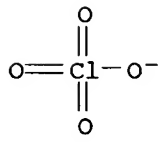


PAGE 2-A



CM 2

CRN 14797-73-0
CMF Cl O4



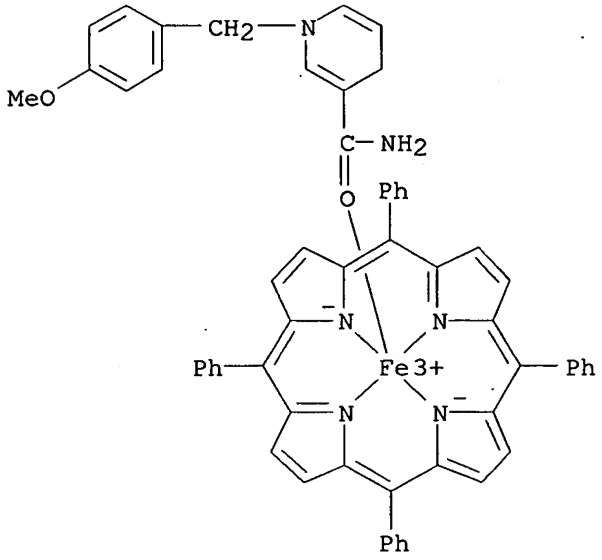
IT **127776-90-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(intramol. electron exchange in, kinetics of)
RN 127776-90-3 HCAPLUS

Delacroix

CN Iron(1+), [1,4-dihydro-1-[(4-methoxyphenyl)methyl]-3-pyridinecarboxamide-O3][5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (SP-5-12)-, perchlorate (9CI) (CA INDEX NAME)

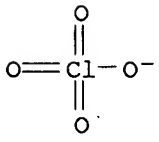
CM 1

CRN 127776-89-0
CMF C58 H44 Fe N6 O2
CCI CCS



CM 2

CRN 14797-73-0
CMF Cl O4



L4 ANSWER 10 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN
AB The mixing of equal vols. of 0.2 mmol dm-3 1-benzylnicotinamide ion and 2 mmol dm-3 cyanide ion results in the immediate formation of a transient absorption band at 375 nm which can be ascribed to a charge-transfer complex. This complex disappears within ca. 0.2 s with the formation of the 1,6-addition product which, in turn, is rapidly converted into the thermodynamically more stable 1,4-adduct. Me substitution at the 6-position of the nicotinamide ring inhibits the formation of the 1,6-adduct, resulting in an increase in the lifetime of the

charge-transfer complex. Subsequently a mixture of the 1,4-cyanide adduct and, most likely, the 1,2-adduct is formed. Rate effects with variation of substituents in the 1-benzyl group reveal that charge-transfer complex formation is counterproductive to the formation of addition products.

1990:422794 Document Number 113:22794 Addition of cyanide ion to nicotinamide cations in acetonitrile. Formation of nonproductive charge-transfer complexes. Engbersen, Johan F. J.; Koudijs, Arie; Sleiderink, Hedwig M.; Franssen, Maurice C. R. (Laboratory Organic Chemical, Agric. University, Wageningen, 6703 HB, Neth.). Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1), 79-83 (English) 1990. CODEN: JCPKBH. ISSN: 0300-9580. OTHER SOURCES: CASREACT 113:22794.

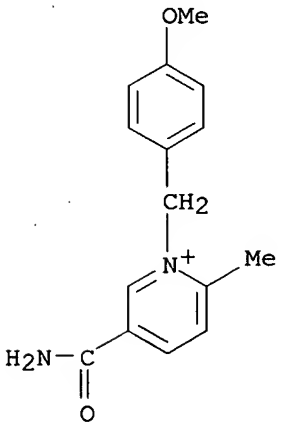
IT **127678-22-2**
RL: PROC (Process)
(decay of, kinetics of)

RN 127678-22-2 HCAPLUS

CN Pyridinium, 5-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-2-methyl-, cyanide (9CI) (CA INDEX NAME)

CM 1

CRN 127678-21-1
CMF C15 H17 N2 O2



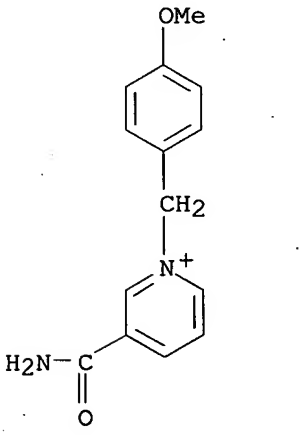
CM 2

CRN 57-12-5
CMF C N

IT **63828-55-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and addition reaction of, with cyanide)

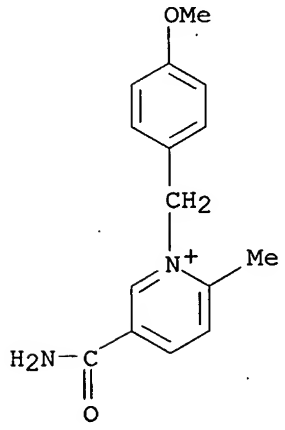
RN 63828-55-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl^-

IT **127663-05-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and charge-transfer complexation of, with cyanide)
RN 127663-05-2 HCAPLUS
CN Pyridinium, 5-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-2-methyl-, chloride (9CI) (CA INDEX NAME)

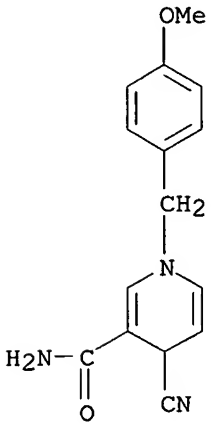


● Cl^-

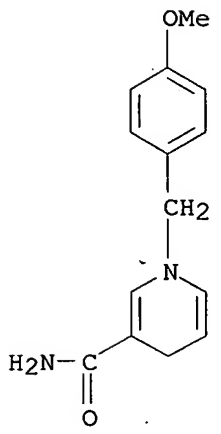
IT **127663-03-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and dissociation of, kinetics of)

Delacroix

RN 127663-03-0 HCAPLUS
CN 3-Pyridinecarboxamide, 4-cyano-1,4-dihydro-1-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 11 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN
AB Electrogenerated chemiluminescence is used to show that the radicals NAD• and NADP• are intermediates in the electrooxidn. of NADH and NADPH at a Pt anode in anhydrous or partly aqueous (up to 15 volume%) DMSO. An ECE mechanism seems to predominate. The use of DMSO proved to be very convenient, with the advantage of enabling electrogenerated chemiluminescence to be obtained in partly aqueous media even with ionic substances as substrates. The method is useful in proving the existence of unstable radical intermediates in redox processes, even for relatively large mols. such as NADH and NADPH.
1988:578804 Document Number 109:178804 Evidence for a radical intermediate in the anodic oxidation of reduced nicotinamide adenine dinucleotides obtained by electrogenerated chemiluminescence. Ludvik, J.; Volke, J. (J. Heyrovsky Inst. Phys. Chemical Electrochem., Czech. Acad. Sci., Prague, 182 23, Czech.). Analytica Chimica Acta, 209(1-2), 69-78 (English) 1988. CODEN: ACACAM. ISSN: 0003-2670.
IT **56133-30-3**
RL: PRP (Properties)
(radical formation in anodic oxidation of, electrochemiluminescence in study of)
RN 56133-30-3 HCAPLUS
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 12 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN

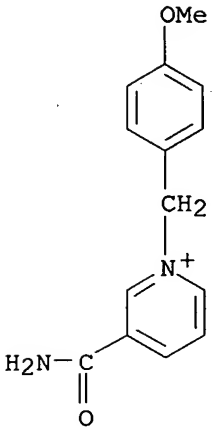
AB The substituent effect (H, NO2, CO2H, Br, Cl, NHAc, Me, OMe, OH, NEt2) on the polarog. behavior of p-substituted 1-phenyl-3-aminocarbonylpyridinium cations has been investigated, in particular on their half-wave potentials in aqueous phosphate buffers pH 6·65 (10% DMF) and in anhydrous solns. of DMF with 0·05 mol L-1 Bu4N+ BF4- as supporting electrolyte. The half-wave potentials of the reduction wave which corresponds to the uptake of a single electron (wave B) and to the formation of the primary radical, obey a Hammett correlation in a way similar to the case of 1-benzyl-3-aminocarbonylpyridinium cations. The slope Qπ,R in the Hammett plot equals 0·093 V for 10% DMF and 0·179 V for anhydrous DMF and compares thus with the slope obtained with the 1-benzyl derivs. where 0.05 V was found for water and 0·127 V of anhydrous acetonitrile. The transfer of the substituent effect from the substituent in the para position on the benzene nucleus to the heterocyclic ring is thus equally active in both substances and depends more strongly on the solvent than on the structure of the cation of both types. The low sensitivity in both series towards a change in the substituent is explained by the fact that during the uptake of the electron the benzene and the pyridine nucleus are not even approx. coplanar. This is why the π-overlap between the two nuclei is considerably restricted. The anal. of sampled d.c.-polarog. waves has confirmed that the one-electron uptake is followed by a chemical reaction, most probably a dimer formation or a reaction of the primary product with the starting substance.

1988:166806 Document Number 108:166806 Polarographic reduction of p-substituted 1-phenyl-3-(aminocarbonyl)pyridinium salts. Krechl, Jiri; Mizaninoiva, Daniela; Volke, Jiri; Kuthan, Josef (Dep. Organic Chemical, Prague Inst. Chemical Technol., Prague, 166 28, Czech.). Collection of Czechoslovak Chemical Communications, 52(6), 1550-60 (English) 1987. CODEN: CCCCAK. ISSN: 0366-547X.

IT **63828-55-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(polarog. reduction of)

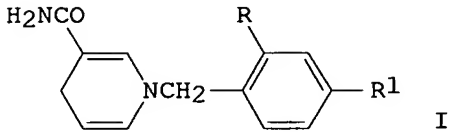
RN 63828-55-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl^-

L4 ANSWER 13 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN
GI



I

AB Stable 6-coordinate high-spin Fe(III) porphyrin complexes with NADH model compds. as ligands were formed in CH2Cl2 containing perchlorato(meso-tetraphenylporphyrinato)iron(III) [FeL(ClO4)] and the NADH model compds. I [R = H, R1 = H (L1), OMe, Me, Cl; R = R1 = Cl] and N-methylacridan. E.g., FeLL1(ClO4) and [FeLL12]+ were formed from FeL(ClO4) and L1 in CH2Cl2. Formation consts. were determined for the complexes and spectroscopic, electrochem., and magnetic properties are reported.

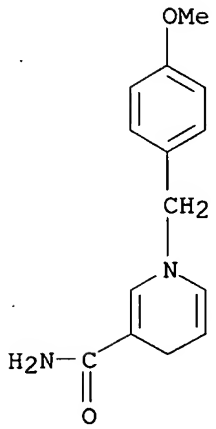
1987:49838 Document Number 106:49838 Six-coordinate high-spin iron(III) porphyrin complexes with NADH model compounds. Fukuzumi, Shunichi; Kondo, Yuji; Tanaka, Toshio (Dep. Appl. Chemical, Osaka University, Osaka, 565, Japan).

Journal of the Chemical Society, Chemical Communications (15), 1053-4 (English) 1985. CODEN: JCCCAT. ISSN: 0022-4936. OTHER SOURCES: CASREACT 106:49838.

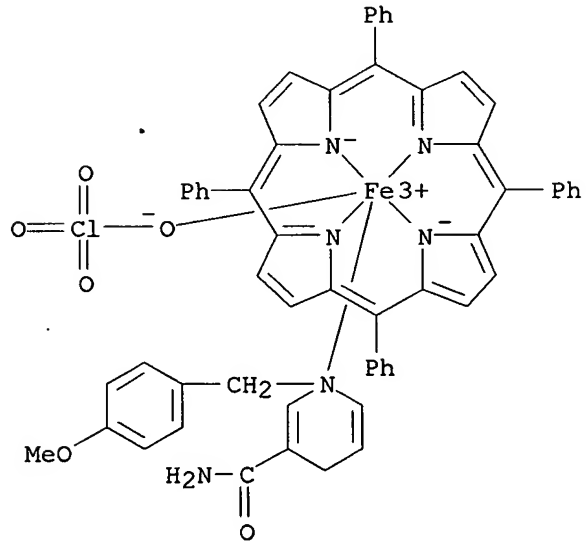
IT **56133-30-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation of, with perchlorato(meso-tetraphenylporphyrinato)iron(III), formation constant for)

RN 56133-30-3 HCAPLUS

CN 3-Pyridinecarboxamide, 1,4-dihydro-1-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



IT **99278-99-6P 99279-01-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and formation constant of)
RN 99278-99-6 HCAPLUS
CN Iron, [1,4-dihydro-1-[(4-methoxyphenyl)methyl]-3-pyridinecarboxamide-N1](perchlorato-O)[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (OC-6-32)- (9CI) (CA INDEX NAME)

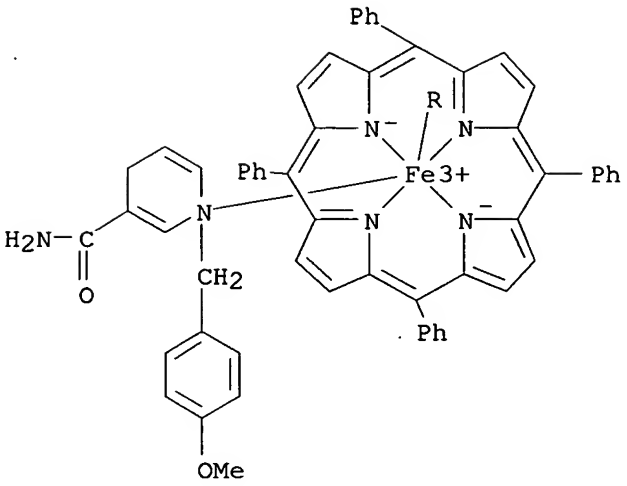


RN 99279-01-3 HCAPLUS
CN Iron(1+), bis[1,4-dihydro-1-[(4-methoxyphenyl)methyl]-3-pyridinecarboxamide-N1][5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (OC-6-12)-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 99279-00-2
CMF C72 H60 Fe N8 O4
CCI CCS

PAGE 1-A



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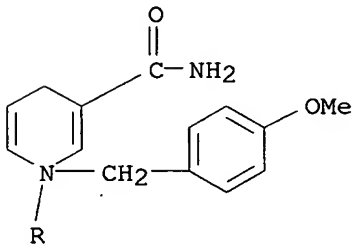
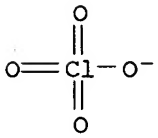


CM 2

CRN 14797-73-0
CMF Cl O4



L4 ANSWER 14 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN
AB Quinolinium, pyridinium, and pyrazinium salts were reduced selectively to 1,4-dihydroquinolines, 1,4-dihydropyridines, and 1,6-dihydropyrazines, resp., by 1-benzyl-1,2-dihydroisonicotinamide (I) in dry MeOH under N. E.g., reduction of N-benzyl-3-carbamoylquinolinium bromide by I for 5 min gave

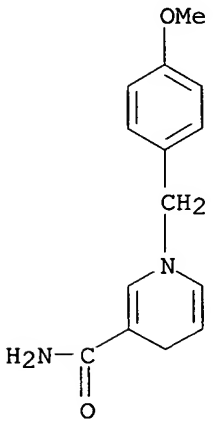
N-benzyl-1,4-dihydroquinoline-3-carboxamide quant.

1985:422428 Document Number 103:22428 Selective reduction of pyridinium, quinolinium, and pyrazinium salts to the dihydro stage with 1-benzyl-1,2-dihydroisonicotinamide. Nuvole, Antonio; Paglietti, Giuseppe; Sanna, Paolo; Acheson, R. Morrin (Ist. Chim. Farm., University Sassari, Sassari, 07100, Italy). Journal of Chemical Research, Synopses (11), 356-7 (English) 1984. CODEN: JRPSDC. ISSN: 0308-2342. OTHER SOURCES: CASREACT 103:22428.

IT **56133-30-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by selective reduction of quaternary compound with benzyldihydroisonicotinamide)

RN 56133-30-3 HCAPLUS

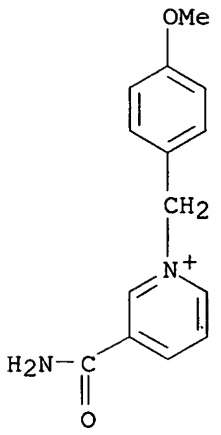
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



IT **63828-55-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by benzyldihydroisonicotinamide, regioselective)

RN 63828-55-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl^-

L4 ANSWER 15 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN

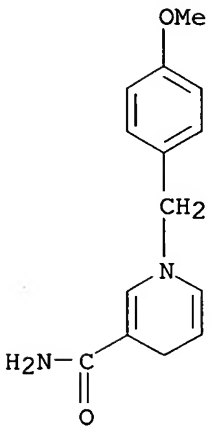
AB Half-wave potentials E1/2 for the electrochem. oxidation of the title heterocycles were measured on a Pt rotating-disc electrode in aqueous and anhydrous DMF; apparent rate consts. k2 of their oxidation with K3Fe(CN)6 were measured in H2O at 298 K. The 2 values (E1/2 and k2) correlated both mutually and with empirical σp substituent consts.

1983:521591 Document Number 99:121591 Dihydropyridines. XLIX. Substituent effects in electrochemical and ferricyanide oxidations of para-substituted 1-benzyl-3-carbamoyl-1,4-dihydropyridines. Pavlikova-Raclova, Frantiska; Kuthan, Josef (Dep. Organic Chemical, Prague Inst. Chemical Technol., Prague, 166 28/6, Czech.). Collection of Czechoslovak Chemical Communications, 48(5), 1408-21 (English) 1983. CODEN: CCCCAK. ISSN: 0366-547X.

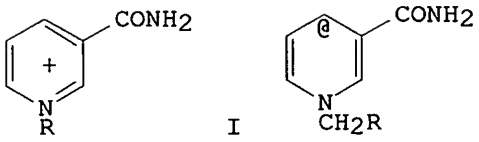
IT **56133-30-3**
RL: PRP (Properties)
(electrochem. and ferricyanide oxidation of, kinetics of)

RN 56133-30-3 HCAPLUS

CN 3-Pyridinecarboxamide, 1,4-dihydro-1-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 16 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN
GI



AB Rate consts. for the title reaction were determined in aqueous solns. of 8 quaternary salts of nicotinamide (I; R = p-XC6H4CH2; X = MeO, Me, H, F,Cl, CO2Me, cyano, NO2). Good Hammett correlations were found, along with correlation of E1/2 of polarog. reduction of I with rate and equilibrium consts.

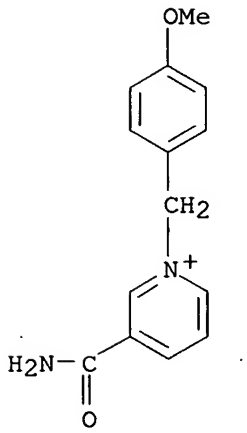
In aqueous media, reduction of I (same R; X = Me, H, F, Cl, MeO) with π-donor substituents proceeds via a simple E mechanism I → II, whereas in the case of π-acceptor substituents (I; X = NO2, CN, CO2Me), radicals II are formed via a 3-step CEC mechanism.

1983:504507 Document Number 99:104507 Dihydropyridines. XLVIII. Substituent effect in addition of cyanide ion to p-substituted 1-benzyl-3-carbamoylpyridinium chlorides. Pavlikova-Raclova, Frantiska; Kuthan, Josef (Dep. Organic Chemical, Prague Inst. Chemical Technol., Prague, 166 28/6, Czech.). Collection of Czechoslovak Chemical Communications, 48(5), 1401-7 (English) 1983. CODEN: CCCCAK. ISSN: 0366-547X.

IT **63828-55-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation of, kinetics and mechanism of)

RN 63828-55-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L4 ANSWER 17 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN

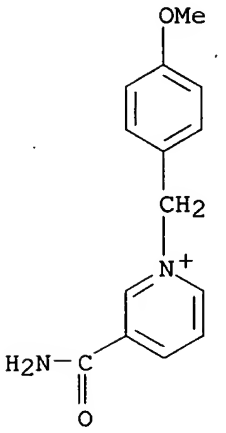
AB Substituent effects (H, NO2, CN, CO2Me, Me, MeO, Me2N, Cl, F) on polarog. characteristics of the title quaternary salts were studied in H2O, anhydrous MeCN, and aqueous EtOH. In the last solvent, 1 of the polarog. waves gradually disappears. The probable course of the investigated electrode processes and accompanying chemical transformations is discussed.

1983:61940 Document Number 98:61940 Polarographic reduction of p-substituted 1-benzyl-3-carbamoylpyridinium chlorides. Kuthan, Josef; Pavlikova-Raclova, Frantiska (Dep. Organic Chemical, Prague Inst. Chemical Technol., Prague, 166 28/6, Czech.). Collection of Czechoslovak Chemical Communications, 47(11), 2890-903 (English) 1982. CODEN: CCCCAK. ISSN: 0366-547X.

IT **63828-55-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, electrochem.)

RN 63828-55-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl^-

L4 ANSWER 18 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN

AB Carboxylate, pyrophosphate, and hydroxyl groups can accelerate the nonenzymic rates of dihydronicotinamide redns. via intramol. noncovalent interactions. The accelerations by the neg. charged carboxylate and pyrophosphate groups occur in nonpolar solvents but the effect of the hydroxyl groups occurs both in aqueous and nonaq. solution The largest effects are observed for neighboring carboxylate groups in nonpolar solvents; e.g., the 2nd-order rate constant for the reduction of N-methylacridinium ion by N-cis-2'-carboxycyclopentyldihydronicotinamide in acetonitrile is 1000-fold more rapid than the rate constant for the corresponding Me ester. Apparently, the neg. charged carboxylate stabilizes the partial pos. charge which develops on the nicotinamide moiety in the transition state. The conclusion that the neg. charged pyrophosphate can enhance dihydronicotinamide redns. is based on the observation that β-NADH reduces N-methylacridinium ion 30-fold faster in MeOH than in aqueous solution, whereas α-NADH reduces the oxidant only 7-fold faster in MeOH than in water. The pyrophosphate group enhances the reaction rates of both anomers by a distance-dependent field effect. The magnitude is greater for the β anomer because the pyrophosphate and nicotinamide moieties are nearer neighbors in this anomer. The rate accelerations produced by hydroxyl groups of alcs. are not as great as those observed for carboxylate groups in nonpolar solvents. In aqueous solns., α-NADH reduces 3 different oxidants 10-fold more rapidly than β-NADH. In acetonitrile, synthetic dihydronicotinamides containing hydroxyl groups increase the rate 6-fold. These modest accelerations with the neutral hydroxyl groups emphasize the importance of a neg. charged group in order to achieve large enhancements in nonaq. solns.

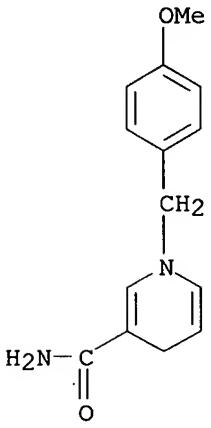
1977:480366 Document Number 87:80366 Model dehydrogenase reactions. Catalysis of dihydronicotinamide reductions by noncovalent interactions. Hajdu, Joseph; Sigman, David S. (Sch. Med., University California, Los Angeles, CA, USA). Biochemistry, 16(13), 2841-6 (English) 1977. CODEN: BICHAW. ISSN: 0006-2960.

IT **56133-30-3**

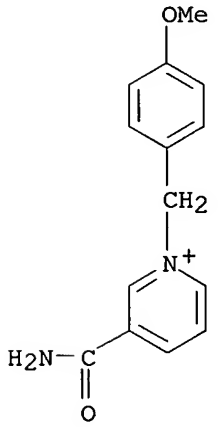
RL: RCT (Reactant); RACT (Reactant or reagent)

(N-methylacridinium reduction by, dehydrogenase reaction mechanism in

relation to)
RN 56133-30-3 HCAPLUS
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



IT **63828-55-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L4 ANSWER 19 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN
AB 2'-Carboxy-N-benzyldihydronicotinamide (I) reduces N-methylacridinium ion 150 times more rapidly than N-benzyldihydronicotinamide in acetonitrile.

Delacroix

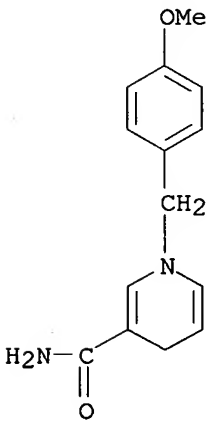
The rate enhancement is only a factor of 3 in aqueous solution The carboxylate group of I most likely enhances the reactivity of this reducing agent in acetonitrile by stabilization of the developing positive charge on the nicotinamide ring in the transition state. These studies provide the 1st example of a noncovalent interaction which is capable of enchancing the reactivity of a dihydronicotinamide. X-ray crystallographic studies of an abortive ternary complex of lactate dehydrogenase have revealed that the carboxylate group of a glutamyl residue is adjacent to the N atom of the nicotinamide ring of the bound coenzyme. The mechanistic role suggested for the carboxylate group in the nonenzymic dihydronicotinamide reaction may be of general importance in the mechanism of action of NAD(P)-dependent dehydrogenases.

1975:455207 Document Number 83:55207 Model dehydrogenase reactions. Neighboring group effects in dihydronicotinamide reductions. Hajdu, Joseph; Sigman, David S. (Sch. Med., University California, Los Angeles, CA, USA). Journal of the American Chemical Society, 97(12), 3524-6 (English) 1975. CODEN: JACSAT. ISSN: 0002-7863.

IT **56133-30-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylacridinium reduction by, kinetics of)

RN 56133-30-3 HCAPLUS

CN 3-Pyridinecarboxamide, 1,4-dihydro-1-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



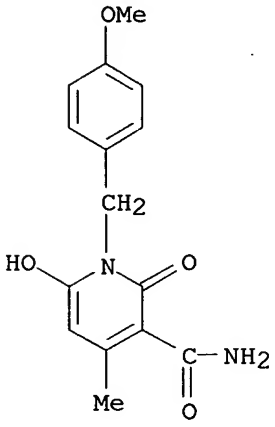
L4 ANSWER 20 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN

AB 1- Or 4-(sulfoaryl)-6-hydroxy-2-pyridinones (I, R = Et or sulfophenyl or sulfobenzyl derivative, R1 = H, CONH2, R2 = Me or sulfophenyl or sulfobenzyl when R = Et) were prepared and were useful as couplers in the manufacture of azo
dyes. Thus, 3-cyano-1-ethyl-4-(p-methoxyphenyl)-6-hydroxypyridin-2-one was added to 96% H2SO4 and heated at 55-60.deg. for 17 hr to give pyridinone coupler (II) [35820-83-8]. The other I were similarly prepared from 3-cyano precursors.

1973:547434 Document Number 79:147434 1 or 4-(Sulfoaryl)-6-hydroxy-2-pyridinones. Austin, Peter W.; Crabtree, Allen (Imperial Chemical Industries Ltd.). U.S. US 3763170 19731002, 3 pp. (English). CODEN: USXXAM. APPLICATION: US 1971-182145 19710920.

IT **49693-68-7P**

RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)
RN 49693-68-7 HCAPLUS
CN Benzenesulfonic acid, 2(or 5)-[[3-(aminocarbonyl)-6-hydroxy-4-methyl-2-oxo-1(2H)-pyridinyl]methyl]-5(or 2)-methoxy- (9CI) (CA INDEX NAME)

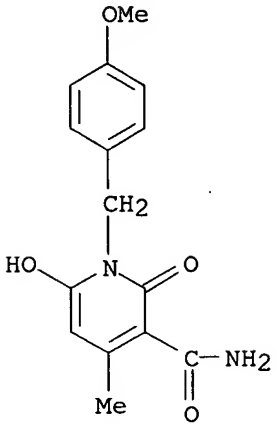


D1—SO3H

L4 ANSWER 21 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN
AB Seven title compds. [I, R = Et, 4-MeO(HO3S)C6H3, 4-HO3SC6H4CH2, 4,3(or 2)-MeO(HO3S)C6H3CH2, or 4,3(or2)-Me(HO3S)C6H3CH2; R1 = H or CONH2; R2 = Me or 4,3-MeO(HO3S)C6H3] or their sulfates, useful as coupling components for azo dyes, were prepared by sulfonating the appropriate phenyl- or benzyl-3-cyano-6-hydroxy-2-pyridones with concentrated or fuming H2SO4. Thus, 3-cyano-1-ethyl-4-(4-methoxyphenyl)-6-hydroxy-2-pyridone was treated with 96% H2SO4 for 17 hr at 55-60.deg. to give a sulfonated pyridone [I, R = Et, R1 = CONH2, R2 = 4,3-MeO(HO3S)C6H3] [35820-83-8].
1972:476687 Document Number 77:76687 Sulfophenyl- and sulfobenzyl-6-hydroxy-2-pyridones. Austin, Peter W.; Crabtree, Allen (Imperial Chemical Industries Ltd.). Ger. Offen. DE 2150817 19720413, 14 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1971-2150817 19711012.
IT **38054-99-8P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)
RN 38054-99-8 HCAPLUS
CN Benzenesulfonic acid, 2(or 5)-[[3-(aminocarbonyl)-6-hydroxy-4-methyl-2-oxo-1(2H)-pyridinyl]methyl]-5(or 2)-methoxy-, sulfate (2:1) (salt) (9CI) (CA INDEX NAME)

CM 1

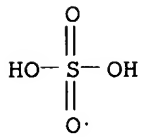
CRN 49693-68-7
CMF C15 H16 N2 O7 S
CCI IDS



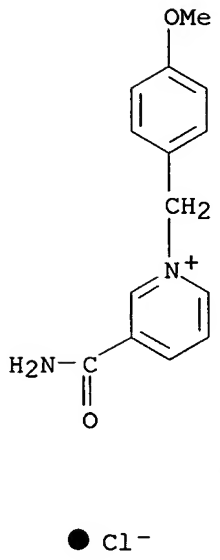
D1—SO_3H

CM 2

CRN 7664-93-9
CMF H2 O4 S



L4 ANSWER 22 OF 22 HCAPLUS COPYRIGHT 2005 ACS on STN
GI For diagram(s), see printed CA Issue.
AB Treatment of 1benzyl-3-carbamoylpyridinium chloride with NaOH in dilute EtOH yielded a new' substance (I), believed to be a cyclic trimer. The structure of I was based on its analysis, infrared spectrum, ultraviolet spectrum, fluorescence spectrum, proton magnetic resonance spectrum, mol. weight, and its chemical reactions. I is believed to have been formed by way of a pyridinium ylide. Several new pseudo base ethers of 1-substituted nicotinamide salts have been prepared
1963:454780 Document Number 59:54780 Original Reference Number 59:9970a-c Action of base on quaternary salts of nicotinamide. Dittmer, Donald C.; Kolyer, J. M. (University of Pennsylvania, Philadelphia). Journal of Organic Chemistry, 28(9), 2288-94 (Unavailable) 1963. CODEN: JOCEAH. ISSN: 0022-3263.
IT **63828-55-7**, Pyridinium, 3-carbamoyl-1-(p-methoxybenzyl)-, chloride (preparation of)
RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)


OMe
CH2
N+
H2N
C
O
Cl-